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Micromechanics Analysis Code (MAC)

User Guide: Version 1.0

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1.0 Introduction

The ability to accurately predict the thermomechanical deformation response of advanced composite materials continues to play an important role in the development of these strategic materials. Analytical models that predict the effective behavior of composites are used not only by engineers performing structural analysis of large-scale composite components but also by material scientists in developing new material systems. For an analytical model to fulfill these two distinct functions it must be based on a micromechanics approach which utilizes physically based deformation and life constitutive models and allows one to generate the average (macro) response of a composite material given the properties of the individual constituents and their geometric arrangement. Only then can such a model be used by a material scientist to investigate the effect of different deformation mechanisms on the overall response of the composite in order to identify the appropriate constituents for a given application. However, if a micromechanical model is to be used in a large-scale structural analysis it must be 1) computationally efficient, 2) able to generate accurate displacement and stress fields at **both** the macro and the micro level and 3) be compatible with the finite element method. Additionally, new advancements in processing and fabrication techniques now make it possible to engineer the architectures of these advanced composite systems. Full utilization of these emerging manufacturing capabilities require the development of a computationally efficient micromechanics analysis tool capable of accurately predicting the effect of microstructural details on the internal and macroscopic behavior of composites. The above mentioned computational efficiency is required since 1) the large number of parameters that must be varied in the course of engineering (or designing) composite materials, and 2) the optimization of a material's microstructure will require the integration of the micromechanics model with optimization algorithms. From this perspective, analytical approaches that produce closed form expressions which describe the effect of a material's internal architecture on the overall material behavior are preferable to numerical methods such as the finite element or finite difference schemes.

A number of models presently exist that can fulfill some aspect of the aforementioned tasks. However, there are very few working models that are both computationally efficient and sufficiently accurate at the micro- as well as the macro-level. One such micromechanics model with the potential of fulfilling both tasks is the method of cells [1] and its generalization [2]. The comprehensive capabilities and efficiency of this method has been documented in references [4] and [5]. Consequently, the recently developed, computationally efficient and comprehensive micromechanics analysis code, **MAC**, whose predictive capability rests entirely upon the fully analytical micromechanics model, herein referred to as the generalized method of cells, GMC, [2 and 3] will now be described. **MAC** is a versatile form of research software that "drives" the double or triply periodic micromechanics constitutive models based upon GMC. GMC is capable of predicting the response of both continuous and discontinuous multi-phased composites with an arbitrary internal microstructure and reinforcement shape. GMC is a continuum based micromechanics model that provides closed-form expressions for the mac-

roscopic composite response in terms of the properties, size, shape, distribution, and response of the individual constituents or phases that make up the material. GMC also utilizes physically based viscoplastic deformation and life models for each constituent. Furthermore, expressions relating the internal stress and strain fields in the individual constituents in terms of the macroscopically applied stresses and strains are also available through strain or stress concentration factors. These expressions make possible the investigation of failure processes at the microscopic level at each step of an applied load history. Similarly, GMC provides the capability of studying the influence of bond strength at the fiber/matrix interface which recently has been shown to be an important damage mechanism.

MAC enhances the basic capabilities of GMC by providing a modular framework wherein 1) various thermal, mechanical (stress or strain control) and thermomechanical load histories can be imposed, 2) different integration algorithms may be selected, 3) a variety of constituent constitutive models may be utilized and/or implemented and 4) a variety of fiber architectures may be easily accessed through their corresponding representative volume elements. Figure 1 illustrates the basic flow diagram for this modular framework. The capabilities for this version of **MAC** are discussed in section 2, whereas theoretical and background information on the basic capabilities itemized above is given in section 3. Section 4 describes how one might use **MAC** and will be the most referred to section in the entire manual. Finally, section 5 gives some insights into the future modifications planned for **MAC**.

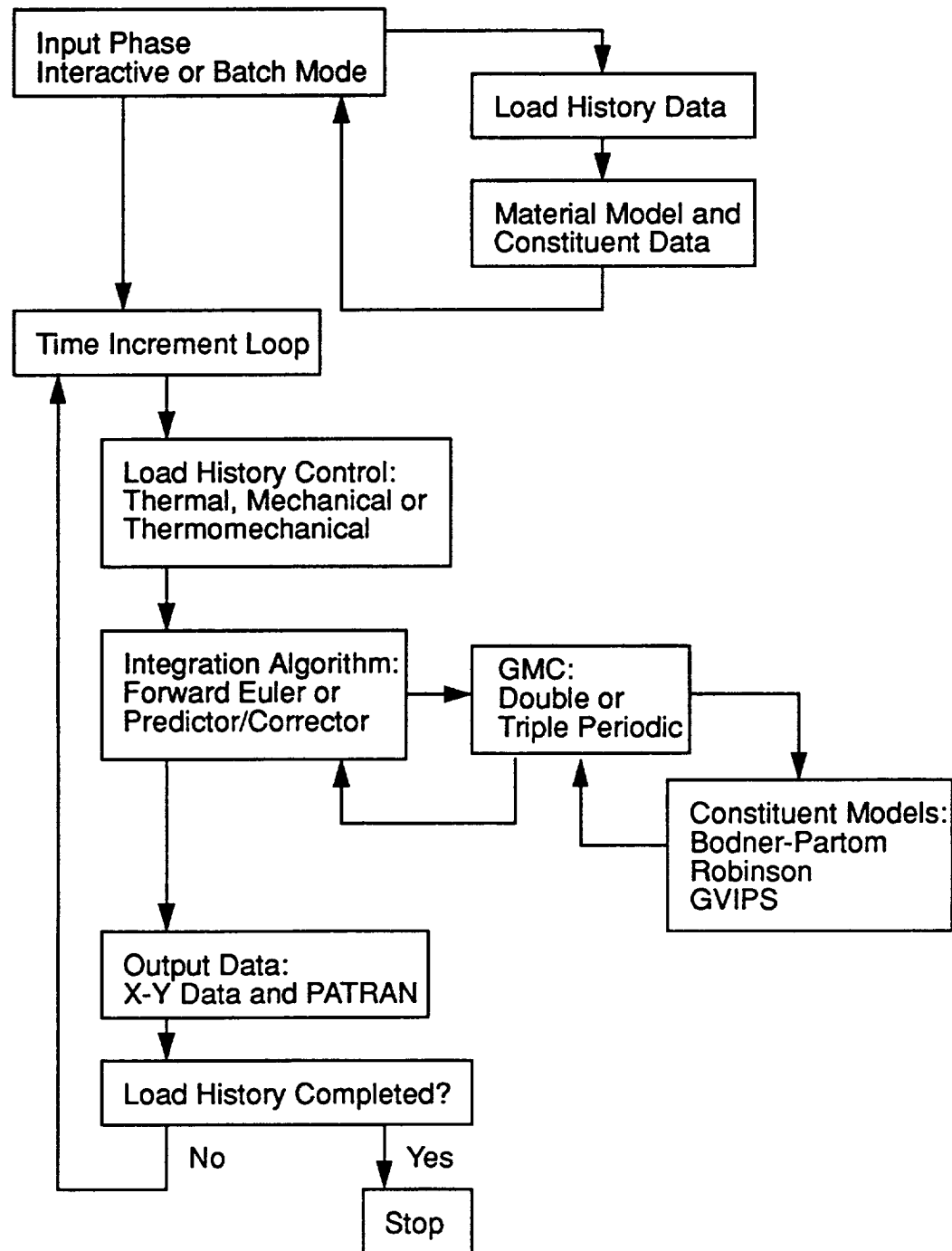


Figure1: **MAC** Flowchart

2.0 Current Capabilities

In this section the current features/capabilities of **MAC** are itemized.

- Load Types:
 - Thermal
 - Mechanical
 - cyclic (stress or strain control)
 - creep (stress control)
 - relaxation (strain control)
 - Thermomechanical
- Aboudi GMC Models:
 - Double Periodicity Model for continuous reinforcement
 - Triple Periodicity Model for discontinuous reinforcement
- Run Options:
 - Interactive
 - Batch
- Graphical Output
 - Up to 5 x-y data plot files may be generated for both macro and micro (sub-cell) quantities
 - PATRAN for subcell geometry and color results evaluation, e.g. stress, strains, inelastic strains, J_2 , etc.
- Integration Options:
 - Forward Euler
 - Predictor/Corrector
- Constitutive Models
 - elastic orthotropic
 - inelastic viscoplastic models:
 - Bodner-Partom
 - Robinson
 - GVIPS

3.0 Background

3.1 Micromechanics Models

As stated in the introduction, **MAC's** predictive capabilities rest entirely upon the fully analytical micromechanics model known as GMC which is capable of predicting the inelastic response of both continuous (double periodicity) and discontinuous (triple periodicity) multi-phased composites with an arbitrary internal microstructure and reinforcement shape. Prior to describing the available architectures (Representative Volume Elements, RVE's) within **MAC** as discussed in section 4, a brief overview of the theoretical foundation behind the generalized method of cells follows. A more complete discussion of the theoretical formulation is given in [1] - [3].

In the original formulation of the method of cells, a continuously (or discontinuously) reinforced, unidirectional fibrous composite is modeled as a rectangular, double-periodic (or triply-periodic) array of fibers embedded in a matrix phase. The periodic character of the assemblage allows one to identify a repeating unit cell that can be used as a building block to construct the entire composite. The properties of the repeating cell are thus representative of the properties of the entire assemblage. The unit cell consists of a single fiber subcell surrounded by three matrix subcells for continuous and seven for discontinuous composites, hence the name **method of cells**. The rectangular geometry of the repeating unit cell allows one to obtain an approximate solution for the stresses and strains in the individual subcells given some macroscopically homogeneous state of strain or stress applied to the composite. The approximate solution to the posed boundary value problem is, in turn, used to determine macroscopic (average) or effective properties of the composite and the effective stress-strain response in the inelastic region.

In the **generalized method of cells** for continuous (or discontinuous) fibrous composites, the repeating unit cell can consist of an arbitrary number of phases. Hence the generalized method of cells is capable of modeling a multiphase composite. This generalization extends the modeling capability of the original method of cells to include the following: 1) inelastic thermomechanical response of multiphased metal matrix composite, 2) modeling of various fiber architectures (including both shape and packing arrangements), 3) modeling of porosities and damage, and 4) the modeling of interfacial regions around inclusions including interfacial degradation.

The basic homogenization approach taken in the micromechanical analysis consists essentially of four steps. First, the repeating volume element, RVE, of the periodic composite is identified. Second, the macroscopic or average stress and strain state in terms of the individual microscopic (subcell) stress and strain states is defined. Third, the continuity of tractions and displacements are imposed at the boundaries between the constituents. These three steps, in conjunction with

micro-equilibrium, establish the relationship between micro (subcell) total, thermal and inelastic strains and macro (composite) strains via the relevant concentration tensors. In the fourth and final step, the overall macro constitutive equations of the composite are determined. These four steps form the basis of the micro-to-macro-mechanics analysis which describe the behavior of heterogeneous media. The resulting micromechanical analysis establishes the overall (macro) behavior of the multi-phase composite and is expressed as a constitutive relation between the average stress, strain, thermal, and inelastic strains, in conjunction with the effective elastic stiffness tensor.

That is,

$$\bar{\sigma} = \underline{B}^* (\bar{\epsilon} - \bar{\epsilon}^I - \bar{\epsilon}^T) \quad (\text{EQ 1})$$

where for the most general case of discontinuous reinforcement with N_α by N_β by N_γ number of subcells, the effective elastic stiffness tensor, \underline{B}^* , of the composite is given by,

$$\underline{B}^* = \frac{1}{dhl} \sum_{\alpha=1}^{N_\alpha} \sum_{\beta=1}^{N_\beta} \sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma \underline{C}^{(\alpha\beta\gamma)} \underline{A}^{(\alpha\beta\gamma)} \quad (\text{EQ 2})$$

the composite inelastic strain tensor is defined as,

$$\bar{\epsilon}^I = \frac{-\underline{B}^{*-1}}{dhl} \sum_{\alpha=1}^{N_\alpha} \sum_{\beta=1}^{N_\beta} \sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma \underline{C}^{(\alpha\beta\gamma)} (\underline{D}^{(\alpha\beta\gamma)} \underline{\epsilon}_s^I - \bar{\epsilon}^I^{(\alpha\beta\gamma)}) \quad (\text{EQ 3})$$

the average thermal strain tensor as,

$$\bar{\epsilon}^T = \frac{-\underline{B}^{*-1}}{dhl} \sum_{\alpha=1}^{N_\alpha} \sum_{\beta=1}^{N_\beta} \sum_{\gamma=1}^{N_\gamma} d_\alpha h_\beta l_\gamma \underline{C}^{(\alpha\beta\gamma)} (\underline{D}^{(\alpha\beta\gamma)} \underline{\epsilon}_s^T - \bar{\epsilon}^T^{(\alpha\beta\gamma)}) \quad (\text{EQ 4})$$

and $\bar{\epsilon}$ is the uniform applied macro (composite) strain. For the case of continuous reinforcements with N_β by N_γ number of subcells, eq. (2) - (4) reduce to the following:

$$\underline{B}^* = \frac{1}{hl} \sum_{\beta=1}^{N_\beta} \sum_{\gamma=1}^{N_\gamma} h_\beta l_\gamma \underline{C}^{(\beta\gamma)} \underline{A}^{(\beta\gamma)} \quad (\text{EQ 5})$$

$$\bar{\epsilon}^I = \frac{-\underline{B}^{*-1}}{hl} \sum_{\beta=1}^{N_\beta} \sum_{\gamma=1}^{N_\gamma} h_\beta l_\gamma \underline{C}^{(\beta\gamma)} (\underline{D}^{(\beta\gamma)} \underline{\epsilon}_s^I - \bar{\epsilon}^I^{(\beta\gamma)}) \quad (\text{EQ 6})$$

$$\bar{\epsilon}^T = \frac{-\underline{B}^{*-1}}{hl} \sum_{\beta=1}^{N_\beta} \sum_{\gamma=1}^{N_\gamma} h_\beta l_\gamma \underline{C}^{(\beta\gamma)} (\underline{D}^{(\beta\gamma)} \underline{\epsilon}_s^T - \bar{\epsilon}^T^{(\beta\gamma)}) \quad (\text{EQ 7})$$

In the above equations matrix notation is employed; where, for example, the average stress, $\bar{\sigma}$, average applied strain, $\bar{\epsilon}$, and inelastic subcell strain, ϵ_s^I , vectors represent,

$$\bar{\sigma} = \{ \bar{\sigma}_{11}, \bar{\sigma}_{22}, \bar{\sigma}_{33}, \bar{\sigma}_{12}, \bar{\sigma}_{23}, \bar{\sigma}_{13} \} \quad (\text{EQ 8})$$

$$\bar{\epsilon} = \{ \bar{\epsilon}_{11}, \bar{\epsilon}_{22}, \bar{\epsilon}_{33}, \bar{\epsilon}_{12}, \bar{\epsilon}_{23}, \bar{\epsilon}_{13} \} \quad (\text{EQ 9})$$

$$\epsilon_s^I = \{ \bar{\epsilon}^{I(111)}, \dots, \bar{\epsilon}^{I(N_\alpha N_\beta N_\gamma)} \} \quad (\text{EQ 10})$$

where the six components of the vector $\bar{\epsilon}^{I(\alpha\beta\gamma)}$ are arranged as in eq. (9). Similar definitions for ϵ_s^T , $\bar{\epsilon}^{T(\alpha\beta\gamma)}$ also exist. Note that the key ingredient in the construction of this macro constitutive law is the derivation of the appropriate concentration matrices, $A^{(\alpha\beta\gamma)}$ and $D^{(\alpha\beta\gamma)}$ having the dimensions 6 by 6 and 6 by $N_\alpha N_\beta N_\gamma$ respectively, at the micro (subcell) level. The definitions of A and D , although not given here, may be found in references [2] and [5]. Finally, the matrix $C^{(\alpha\beta\gamma)}$ represents the elastic stiffness tensor of each subcell $(\alpha\beta\gamma)$ and d_α , h_β , l_γ the respective subcell dimensions (see Fig. 2) wherein,

$$d = \sum_{\alpha=1}^{N_\alpha} d_\alpha \quad h = \sum_{\beta=1}^{N_\beta} h_\beta \quad l = \sum_{\gamma=1}^{N_\gamma} l_\gamma$$

Similarly, given the concentration matrices $A^{(\alpha\beta\gamma)}$ and $D^{(\alpha\beta\gamma)}$, expressions for the average strain in each subcell can be constructed, i. e.,

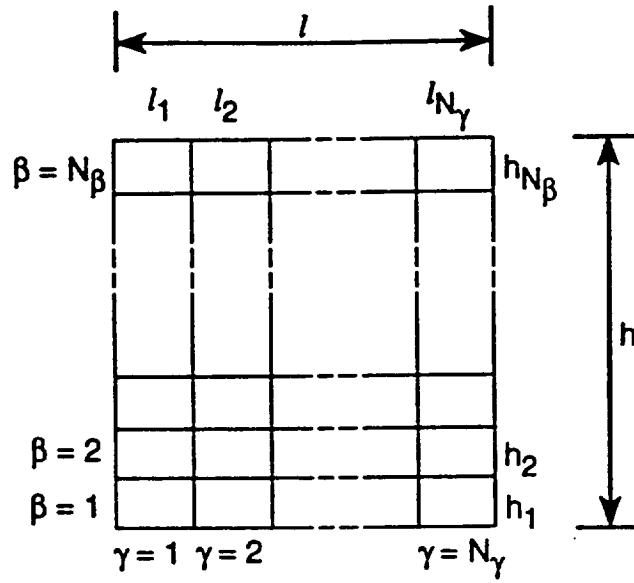
$$\bar{\epsilon}^{(\alpha\beta\gamma)} = A^{(\alpha\beta\gamma)} \bar{\epsilon} + D^{(\alpha\beta\gamma)} (\epsilon_s^I + \epsilon_s^T)$$

as well as average stress,

$$\bar{\sigma}^{(\alpha\beta\gamma)} = C^{(\alpha\beta\gamma)} [A^{(\alpha\beta\gamma)} \bar{\epsilon} + D^{(\alpha\beta\gamma)} (\epsilon_s^I + \epsilon_s^T) - (\epsilon^{I(\alpha\beta\gamma)} + \epsilon^{T(\alpha\beta\gamma)})]$$

The analytic constitutive law, see eq. 1, may be readily applied to investigate the behavior of various types of composites, given knowledge of the behavior of the individual phases. Numerous advantages can be stated regarding the current macro/micro constitutive laws as compared to the other numerical micromechanical approaches in the literature, e.g. the finite element unit cell approach. One advantage is that any type of simple or combined loading (multiaxial state of stress) can be applied irrespective of whether symmetry exists or not, as well as without resorting to different boundary condition application strategies as in the case of the finite element unit cell procedure. Another, advantage concerns the

Double
Periodicity



Triple
Periodicity

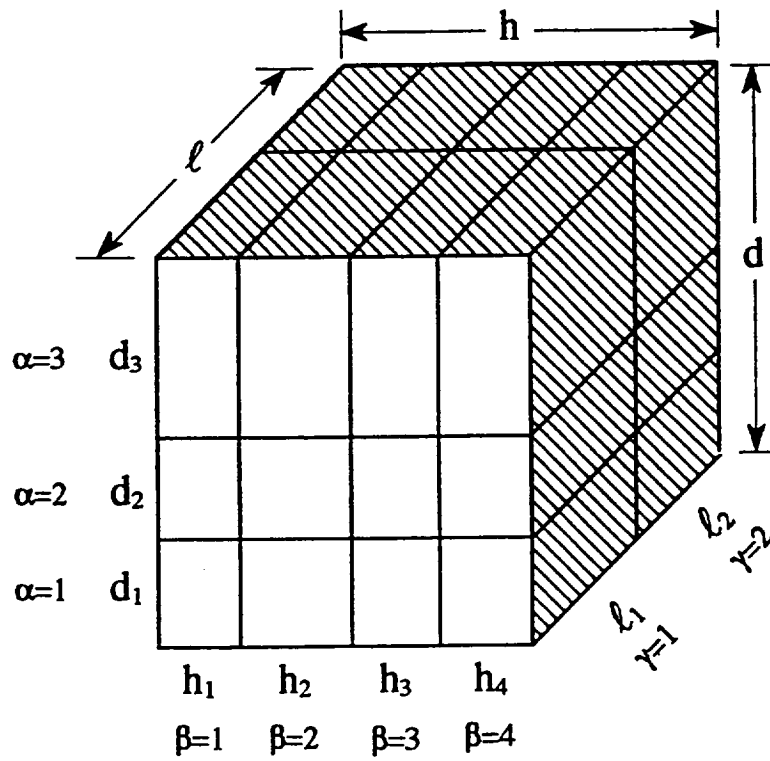


Figure 2: Subcell Dimension Nomenclature

availability of an analytical expression representing the macro elastic-thermo-inelastic constitutive law thus ensuring a reduction in memory requirements when implementing this formulation into a structural finite element analysis code. Furthermore, this formulation has been shown to predict accurate macro behavior given only a few subcells, within the repeating cell (see references [2], and [4]). Whereas, if one employs the finite element unit cell procedure, a significant number of finite elements are required within a given repeating unit cell to obtain the same level of accuracy as with the present formulation. Consequently, it is possible to utilize this formulation to efficiently analyze metal matrix composite structures subjected to complex thermomechanical load histories. This is particularly important when analyzing realistic structural components, since different loading conditions exist throughout the structure, thus necessitating the application of the macromechanical equations repeatedly at these locations.

3.2 Integration Algorithms

There are two integration algorithms currently available within **MAC**. The first is the standard, explicit Forward Euler algorithm, which can be expressed as,

$$w_{i+1} = w_i + \Delta t f(t_i, w_i)$$

where

$$\begin{aligned} w_i &= \underline{y}(t_i) \\ w_{i+1} &= \underline{y}(t_{i+1}) \end{aligned}$$

and $f(t_i, w_i)$ is the rate of change with respect to time of the vector, $\underline{y}(t_i)$, i.e.

$$f(t_i, w_i) = \dot{\underline{y}} = \frac{d\underline{y}(t_i)}{dt}$$

The second is a predictor/corrector algorithm which uses:

- 1) a 4th order Runge-Kutta starter:

$$w_i = w_{i-1} + \frac{(K_1 + 2K_2 + 2K_3 + K_4)}{6}$$

where

$$\begin{aligned}
K_1 &= \Delta t f(t_{i-1}, w_{i-1}) \\
K_2 &= \Delta t f(t_{i-1} + \frac{\Delta t}{2}, w_{i-1} + \frac{K_1}{2}) \\
K_3 &= \Delta t f(t_{i-1} + \frac{\Delta t}{2}, w_{i-1} + \frac{K_2}{2}) \\
K_4 &= \Delta t f(t_{i-1} + \Delta t, w_{i-1} + K_3)
\end{aligned}$$

2) with an Adams Bashforth four-step predictor:

$$\begin{aligned}
w_0 &= \alpha_1 & w_1 &= \alpha_2 & w_2 &= \alpha_3 & w_3 &= \alpha_4 \\
w_{i+1}^P &= w_i + \frac{\Delta t}{24} [55f(t_i, w_i) - 59f(t_{i-1}, w_{i-1}) + 37f(t_{i-2}, w_{i-2}) \\
&\quad - 9f(t_{i-3}, w_{i-3})]
\end{aligned}$$

and 3) an Adams Moulton four step corrector:

$$\begin{aligned}
w_{i+1}^C &= w_i + \frac{\Delta t}{24} [9f(t_{i+1}, w_{i+1}^P) + 19f(t_i, w_i) - 5f(t_{i-1}, w_{i-1}) \\
&\quad + f(t_{i-2}, w_{i-2})]
\end{aligned}$$

where the α 's come from the 4th order Runge-Kutta starter. Further details may be found in [6].

It has been found, based on experience, that for relatively rapid monotonic or cyclic loadings it may be more efficient to use the Forward Euler integrator since the predictor/corrector requires 5 evaluations per step, as shown above. However, in the case of creep, relaxation or slow monotonic or cyclic loading histories, significant increases in solution speeds can be obtained using the predictor/corrector algorithm with a self-adaptive time step.

Finally, within **MAC** the vector \underline{y} as used above contains the following macro quantities:

<u>position</u>	<u>contents</u>
1 - 6	Macro Total Strain
7 - 12	Macro Stress
13 - 18	Macro Inelastic Strain
19 - 30	(currently empty space for 2 6x1 vectors)
31 - 36	Macro Thermal Strain
37	Current Temperature

and the quantities associated with each subcell are stored sequentially in \underline{y} , such that

<u>position</u>	<u>contents</u>
38 - 43	Micro Total Strain
44 - 49	Micro Stress
50 - 55	Micro Inelastic Strain
56 - 67	Micro Internal State Variables (space for 2 6x1 vectors)
68 - 73	Micro Thermal Strain

The above 36 positions are repeated for the total number of (N) subcells thus bringing the total length of the \underline{y} vector to 37+36N. It follows that a second vector of similar length contains the corresponding macro and micro rates $\dot{\underline{y}}$.

3.3 Available Constituent Constitutive Models

Currently **MAC** provides four inelastic constitutive models. These models have been selected purely based upon the availability of material parameters for the materials of interest. However, **MAC** is designed in a modular fashion thus allowing the implementation of additional inelastic models. Two of the four available models are capable of representing transversely isotropic material behavior, thus allowing one to investigate the reinforcement of an anisotropic matrix or the idealization of an anisotropic fiber. In all cases a purely elastic response is possible by modifying a single material parameter for each model as noted below.

3.3.1 Bodner-Partom Model

Reference: Mechanics of Composite Materials, Jacob Aboudi, Elsevier, 1991

This model represents the Bodner-Partom viscoplastic model with isotropic hardening, Z , and can be used for an initially isotropic metallic material.

The flow law is given as:

$$\dot{\epsilon}_{ij}^I = \Lambda s_{ij}$$

where

$$\Lambda = \sqrt{\frac{D_2^{PL}}{J_2}}$$

$$D_2^{PL} = D_0^2 \exp \left[- \left(\frac{A^2}{J_2} \right)^n \right]$$

$$A^2 = \frac{1}{3} Z_{eff}^2 \left(\frac{n+1}{n} \right)^{\frac{1}{n}}$$

$$J_2 = \frac{1}{2} S_{ij} S_{ij}$$

$$S_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij}$$

The evolution law for isotropic hardening is given as:

$$\dot{Z} = m (Z_1 - Z_{eff}) \frac{\dot{W}^{PL}}{Z_0}$$

where Z_0 , Z_1 and m are inelastic constants and the plastic work rate, \dot{W}^{PL} , is given by;

$$\dot{W}^{PL} = \sigma_{ij} \dot{\epsilon}_{ij}^I$$

$$Z_{eff} = Z_0 + q \int_0^t \dot{Z}(\tau) d\tau + (1-q) \sum_{i,j=1}^3 r_{ij} \int_0^t \dot{Z}(\tau) r_{ij}(\tau) d\tau$$

$$r_{ij}(t) = \sigma_{ij}(t) / [\sigma_{kl}(t) \sigma_{kl}(t)]^{1/2}$$

An elastic only response may be obtained by setting the material parameter D_0 to zero.

3.3.2 Robinson Creep Model

Reference: NASA TM 103172, 1990

This model represents a transversely isotropic material, wherein the vector of direction cosines, d_i defines the strong material direction along which no inelasticity occurs.

Flow Law:

$$\frac{\dot{\epsilon}_{ij}^I}{\dot{\epsilon}_0} = 2F^n \frac{\Gamma_{ij}}{\sigma_0 \sqrt{F}}$$

Evolution Law:

$$\dot{a}_{ij} = \frac{H}{G^\beta} \frac{1}{2} \frac{\dot{\epsilon}_{ij}^I}{\dot{\epsilon}_0} - R G^{m-\beta} \frac{\Pi_{ij}}{\sigma_0 \sqrt{G}}$$

where

$$\Gamma_{ij} = \Sigma_{ij} - \frac{1}{2} I (3D_{ij} - \delta_{ij})$$

$$\Pi_{ij} = a_{ij} - \frac{1}{2} \hat{I} (3D_{ij} - \delta_{ij})$$

in which

$$F = \frac{4}{\sigma_0^2} \phi \quad \phi = J_2 - \frac{3}{4} I^2$$

$$G = \frac{4}{\sigma_0^2} \psi \quad \psi = \hat{J}_2 - \frac{3}{4} \hat{I}^2$$

and

$$J_2 = \frac{1}{2} \Sigma_{ij} \Sigma_{ji} \quad I = D_{ij} \Sigma_{ji} \quad D_{ij} = d_i d_j \quad \Sigma_{ij} = S_{ij} - a_{ij}$$

$$\hat{J}_2 = \frac{1}{2} a_{ij} a_{ji} \quad \hat{I} = D_{ij} a_{ji} \quad S_{ij} = \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij}$$

Special cases involving an isotropic material can be obtained by defining $d_i = (1/3, 1/3, 1/3)$ and/or elastic only response by setting σ_0 to an extremely large number.

3.3.3 Robinson Viscoplastic Model

Reference: NASA TM 105819, 1992

This model represents a transversely isotropic material wherein the vector of direction cosines d_i defines the preferred material direction. In this model the strength of anisotropy is specified by the parameters ω and η ; where ω is the ratio of the normal longitudinal and transverse yield stress and η is the ratio of longitudinal and transverse shear strengths.

Flow Law:

$$\dot{\epsilon}_{ij}^I = \frac{\langle F^n \rangle}{2\mu} \Gamma_{ij}$$

Evolution Law

$$\dot{a}_{ij} = \frac{H}{G^\beta} \dot{\epsilon}_{ij}^I - R G^{m-\beta} \Pi_{ij}$$

where

$$\Gamma_{ij} = \Sigma_{ij} - \xi (D_{ki} \Sigma_{jk} + D_{jk} \Sigma_{ki} - 2I_0 D_{ij}) - \frac{1}{2} \zeta I_0 (3D_{ij} - \delta_{ij})$$

$$\Pi_{ij} = a_{ij} - \xi (D_{ki} a_{jk} + D_{jk} a_{ki} - 2\hat{I}_0 D_{ij}) - \frac{1}{2} \zeta \hat{I}_0 (3D_{ij} - \delta_{ij})$$

and

$$F = \frac{1}{\kappa_T^2} \left[I_1 + \frac{1}{\eta^2} I_2 + \frac{9}{4(4\omega^2 - 1)} I_3 \right] - 1$$

$$\hat{G} = \frac{1}{\kappa_T^2} \left[\hat{I}_1 + \frac{1}{\eta^2} \hat{I}_2 + \frac{9}{4(4\omega^2 - 1)} \hat{I}_3 \right]$$

$$G = \langle \hat{G} - \hat{G}_0 \rangle H \nu [S_{ij} \pi_{ij}] + \hat{G}_0$$

$$I_1 = J_2 - I - \frac{1}{4} I_3 \quad I_2 = I - I_3 \quad I_3 = I_0^2$$

$$J_2 = \frac{1}{2} \Sigma_{ij} \Sigma_{ji} \quad I = D_{ij} \Sigma_{ji} \quad D_{ij} = d_i d_j \quad \Sigma_{ij} = S_{ij} - a_{ij}$$

$$\xi = \frac{\eta^2 - 1}{\eta^2} \quad \zeta = \frac{4(\omega^2 - 1)}{4\omega^2 - 1}$$

The invariants $\hat{I}_1, \hat{I}_2, \hat{I}_3$ are the same as those given above but with Σ_{ij} replaced by a_{ij} . Special cases involving an isotropic material and/or elastic only response can be obtained by defining $\omega = \eta = 1$ and/or by setting κ_T to an extremely large number.

3.3.4 Generalized Viscoplastic Potential Structure (GVIPS) Model

Reference: NASA TM 106609, 1994

This model is a fully associative, multiaxial, isothermal, nonlinear kinematic hardening viscoplastic model for use with initially isotropic metallic materials. A unique aspect of this model is the inclusion of non-linear hardening through the use of a compliance operator Q_{ijkl} in the evolution law for the back stress. This non-linear tensorial operator is significant in that it allows both the flow and evolutionary laws to be fully associative (and therefore easily integrated) and greatly influences the multiaxial response under non-proportional loading paths.

Flow Law:

$$\dot{\epsilon}_{ij}^I = \frac{3}{2} \|\dot{\epsilon}_{ij}^I\| \frac{\Sigma_{ij}}{\sqrt{J_2}} \quad \text{if} \quad F \geq 0$$

where

$$\|\dot{\epsilon}_{ij}^I\| = \sqrt{\frac{2}{3} \dot{\epsilon}_{ij}^I \dot{\epsilon}_{ij}^I} = \frac{\mu F^n}{\kappa}$$

Internal constitutive rate equation

$$\dot{a}_{ij} = L_{ijrs} \dot{A}_{rs}$$

Evolution Law:

$$\begin{aligned} \dot{A}_{rs} &= \dot{\epsilon}_{rs}^I - \frac{3}{2} \frac{\beta}{\kappa} \|\dot{\epsilon}_{ij}^I\| \frac{a_{rs}}{\sqrt{G}} H\nu[Y] - \frac{3R_\alpha B_0 G^q}{\kappa^2} a_{rs} \quad \text{if} \quad a_{ij} \Sigma_{ij} \geq 0 \\ \dot{A}_{rs} &= Q_{rslm} E_{lmnp} \left(\dot{\epsilon}_{np}^I - \frac{3}{2} \frac{\beta}{\kappa} \|\dot{\epsilon}_{ij}^I\| \frac{a_{np}}{\sqrt{G}} H\nu[Y] - \frac{3R_\alpha B_0 G^q}{\kappa^2} a_{np} \right) \quad \text{if} \quad a_{ij} \Sigma_{ij} < 0 \end{aligned}$$

where

$$F = \left\langle \frac{\sqrt{J_2}}{\kappa} - Y \right\rangle$$

$$Y = \langle 1 - \beta \sqrt{G} \rangle$$

$$G = \frac{I_2}{\kappa^2}$$

$$L_{ijrs} = [Q_{ijrs}]^{-1} = \frac{\kappa^2}{3B_0(1+B_1pG^{p-1})} \left(I_{ijrs} - \frac{3B_1(p-1)G^{p-2}}{\kappa^2(1+B_1pG^{p-1}(6p-5))} a_{rs}a_{ij} \right)$$

and

$$\begin{aligned} I_2 &= \frac{3}{2} a_{ij} a_{ij} & \Sigma_{ij} &= S_{ij} - a_{ij} \\ J_2 &= \frac{3}{2} \Sigma_{ij} \Sigma_{ij} & S_{ij} &= \sigma_{ij} - \frac{1}{3} \sigma_{kk} \delta_{ij} \end{aligned}$$

The special case of an elastic only response maybe obtained by setting κ to an extremely large value.

3.4 References

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- 2) Paley, M., and Aboudi, J.; "Micromechanical Analysis of Composites by the Generalized Method of Cells Model", *Mechanics of Materials*, Vol. 14, pp 127-139, 1992.
- 3) Aboudi, J.; "Micromechanical Analysis of Thermo-Inelastic Multiphase Short-Fiber Composites", NASA CR 195290, 1994.
- 4) Arnold, S.M., Wilt, T.E., Saleeb, A.F., and Castelli, M.G., "An Investigation of Macro and Micromechanical Approaches for a Model MMC System", NASA CP 19117, Vol. II, pp. (52.1) - (52.12), 1993.
- 5) Arnold, S.M., Wilt, T.E., and Pindera, M.J., "Influence of Fiber Architecture on the Elastic and Inelastic Response of Metal Matrix Composites", NASA TM 106705, 1994.
- 6) Burden, R.L. and Faires, J.D.; Numerical Analysis, Prindle, Weber and Schmidt, 1985.
- 7) W.K. Binienda, D.N. Robinson, S.M. Arnold, and P.A. Bartolotta, "A Creep Model for Metallic Composites Based on Matrix Testing: Application to Kanthal Composites", NASA TM 103172, 1990.
- 8) S.M. Arnold, D.N. Robinson, and P.A. Bartolotta, "Unified Viscoplastic Behavior of Metal Matrix Composites", NASA TM 105819, 1992.
- 9) S.M. Arnold, A.F. Saleeb, and M.G. Castelli, "A Fully Associative, Non-Linear Kinematic, Unified Viscoplastic Model for Titanium Based Matrices", NASA TM 106609, 1994.

4.0 Running MAC

MAC provides the user with the option of either running the code in a interactive or batch mode. In the interactive mode, the user is prompted for all necessary input through a series of questions. This mode is most useful for beginners or when solution of a single problem is desired. Execution in the batch or back-ground mode requires the user to construct an input file containing the required input as discussed below. This mode is extremely helpful when performing parametric studies in which only a single parameter is being varied. Since the input requirements for both modes are identical and the interactive input is self explanatory, only the batch mode input requirements will be presented in detail. First, however, a description of the various files required and generated by **MAC** will be given followed by the actual commands required to commence execution of **MAC**.

4.1 MAC Input and Output Files

Input

mac.key

Output

batch.out

PATRAN files (optional, see section 4.3.11)

plot data files (see section 4.3.19)

4.2 Interactive/Batch Mode Execution

Prior to executing **MAC** the mac.key file must exist. The following is an example of the minimum size (3 lines) mac.key file required to run **MAC** in the **interactive** mode.

Required input:

```
first line:      *problem title
second line:    *JRUN interactive=1 batch=2
third line:      1
```

See Appendix A for a sample mac.key file for running in the **batch** mode. Each control block necessary for running in batch mode is described sequentially in the next section.

MAC has been developed for a Sun IPX workstation running Sun OS 4.1.3. Upon linking the associated object modules that comprise **MAC**, execution is begun by simply typing MAC (in upper case) and hitting return.

4.3 Input Requirements: Batch Mode

The following data should appear in the file: mac.key. This mac.key file is the job control data file that is read when the batch mode option is used. Since this file is read sequentially, the data **must** appear in the order given here. Also, note that the key file must exist and the first two command blocks **must always** be included in this key file, i.e. the **Header Line** and **Run Mode** blocks as it will define the execution option for **MAC**.

Note in the following, each block of input data will have its own subsection and will typically contain the following information:

- 1) statement of purpose
- 2) declaration of input block
- 3) example
- 4) notes

☞ **Note:** Each data block contains the line:

***** *comments*

This line **is required** but the actual text, including the ***** , are currently **not** used by the code. The present purpose of this line is to make the mac.key file easier to organize and read.

4.3.1 Header Line:

Purpose: Define the title of this particular job (80A format).

☛ **Note:** the **Header Line** is limited to one line:

* *problem title*

Example: *Transverse tensile response of 35% SCS6/Ti--6-4

4.3.2 Run Mode:

Purpose: To select either the interactive or batch mode of **MAC**.

* *run mode comment*

jrun

jrun:

1 - Interactive mode

2 - Batch mode

Example: (to select batch mode)

*JRUN interactive=1 batch=2

2

4.3.3 Output Print Level:

Purpose: To control the output generated

* *output comment*

nplvl

nplvl:

-1 = print out macro stiffness matrix, engineering constants and macro thermal expansion coefficients

0 = minimal output (most commonly used)

3 = basic program trace

5 = *program execution trace and all array data*

WARNING: *this generates a very large output file*

☛ **Note:** When using the batch mode, all output is written to the file, batch.out. For the interactive mode, all output is written to the screen.

Example: (minimal print out)

*NPLVL

0

4.3.4 Load Type:

Purpose: To select load type

** load type comment*

nse1

nse1:

1 = Thermal Load

2 = Mechanical Load

3 = Thermomechanical Load

Example: (run mechanical load)

*NSEL

2

☛ **Note:** This is where the data would begin if the new problem option is chosen in section 4.3.20

4.3.5 Load Component:

☛ **Note:** This data block is NOT TO BE USED if NSEL = 1 (thermal load)

Purpose: To select the load component (refer to figure 3 for coordinate system to be activated)

** load component comment*

lop

lop:

1 = axial load in 1-direction

2 = axial load in 2-direction

3 = axial load in 3-direction

4 = shear load 12-direction

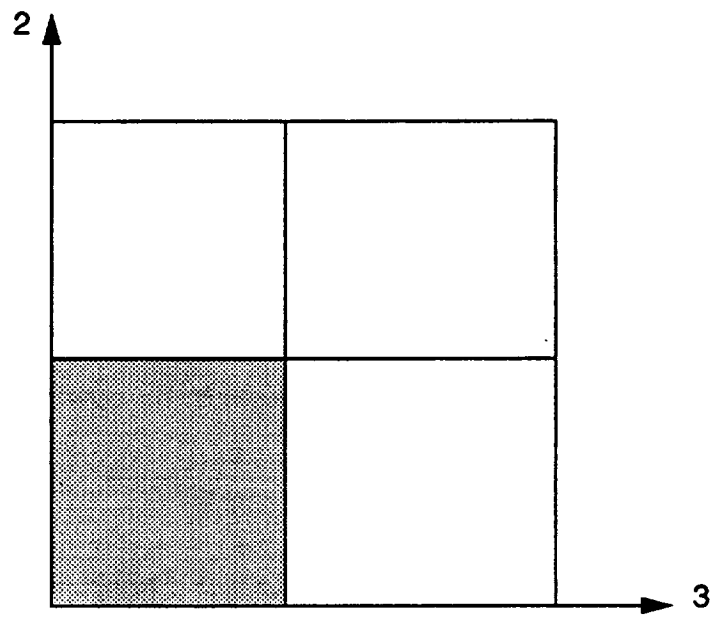
5 = shear load 23-direction

6 = shear load 13-direction

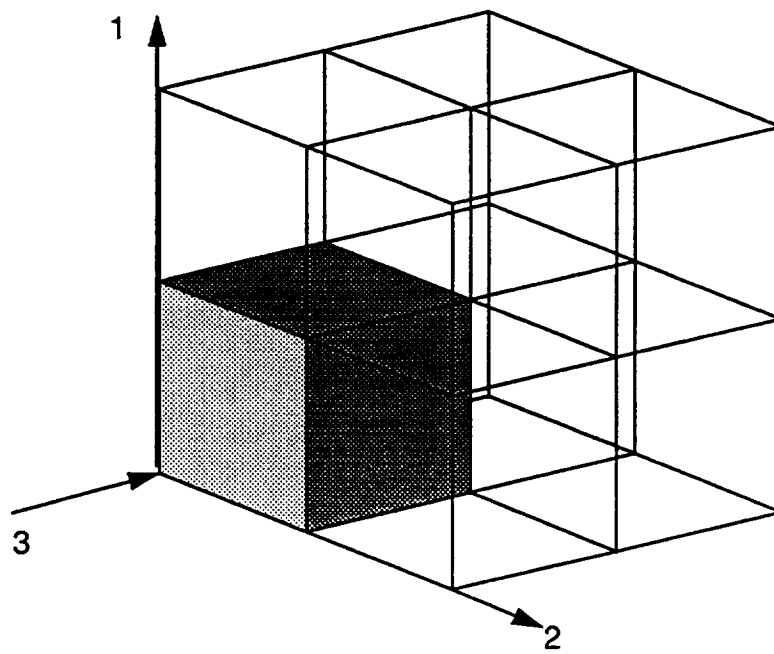
Example: (axial load in 1-direction)

*LOP

1



Double Periodicity



Triple Periodicity

Figure 3: Coordinate Systems

4.3.6 Load Control:

Note: This block is only required if NSEL = 2 or 3

Purpose: Select type of load control for mechanical load

** load control comment*

iopt2

iopt2:

1 = Strain control

2 = Stress control

Example: (strain control)

*IOPT2

1

For Thermal Load (NSEL = 1):

* number of time and temperature points comment
 n_{ptt}
 * time points comment
 $t_1, t_2, \dots, t_{n_{ptt}}$
 * temperature points comment
 $T_1, T_2, \dots, T_{n_{ptt}}$

For Mechanical Load (NSEL = 2):

* number of time and load points comment
 n_{ptw}
 * time points comment
 $t_1, t_2, \dots, t_{n_{ptw}}$
 * load points comment
 $L_1, L_2, \dots, L_{n_{ptw}}$

For Thermomechanical Load (NSEL = 3):

* number of time and load points comment
 n_{ptw}
 * time points comment
 $t_1, t_2, \dots, t_{n_{ptw}}$
 * load points comment
 $L_1, L_2, \dots, L_{n_{ptw}}$
 * number of time and temperature points comment
 n_{ptt}
 * time points comment
 $t_1, t_2, \dots, t_{n_{ptt}}$
 * temperature points comment
 $T_1, T_2, \dots, T_{n_{ptt}}$

n_{pt}, n_{ptw}, n_{ptt} : number of points on load and/or temperature curve(s)

t_1, t_2, \dots : time values

L_1, L_2, \dots : load curve values

T_1, T_2, \dots : temperature curve values

⚠ **Note:** For the Thermomechanical Load $t_{n_{ptw}} \equiv t_{n_{ptt}}$, and both curves must have $t_1 \equiv 0$. But the number and time value of the data points in-between maybe different, see figure 4.

Examples:

For thermal load only analysis (NSEL = 1), using 4 time and temperature points:

```
* NPT
4
* TIME
0., 1., 2., 3.
* TEMPERATURE
0., 100., 200., 300.
```

For mechanical load only analysis (NSEL = 2), using 4 time and load points:

```
* NPT
4
* TIME
0., 1., 2., 3.
* LOAD
0., 10., 20., 30.
```

For thermomechanical load analysis (NSEL = 3), using 4 points for both load and temperature data:

```
* NPTW
4
* TIME
0., 1., 2., 3.
* LOAD
0., 10., 20., 30.
* NPTT
4
* TIME
0., 1., 2., 3.
* TEMPERATURE
0., 100., 200., 300.
```

☛ **Note:** Units must be consistent with selected material model parameter units (4.3.14)
See figure 4 for sketch of load history.

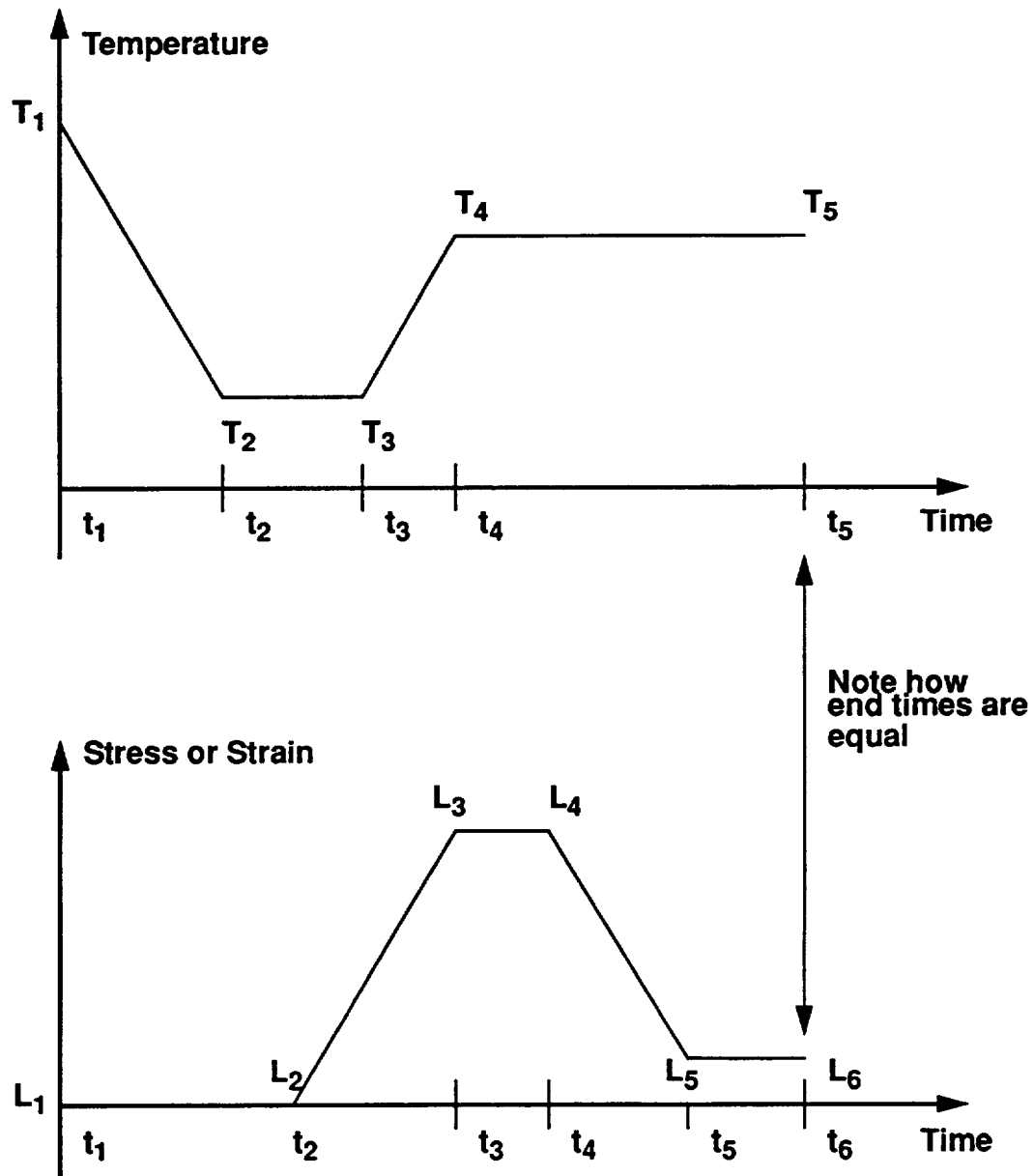


Figure 4: Load History Specification

4.3.8 Reference Temperature:

Purpose: Define initial (starting) temperature

* *reference temperature comment*

tref

tref:

--- temperature

Example: (set reference temperature at 70.)

*TREF

70.

☞ **Note:** only important in thermal or thermomechanical load case when using secant values of coefficient of thermal expansion.

☞ **Note:** Units must be consistent with selected material model parameter units

4.3.9 Micromechanics Model Identification:

Purpose: Select desired GMC micromechanics model

** micromechanics model comment
modid*

modid:

1 = double periodicity (continuous reinforcement)

2 = triple periodicity (discontinuous reinforcement)

Example: (select double periodicity model)

*MODID

1

⚡ **Note:** This is where the data would begin if a new case option is chosen in section 4.3.20

4.3.10 PATRAN Output:

Purpose: To select PATRAN output file generation.

* *PATRAN comment*

patran

prefix

patran:

y = yes, generate PATRAN files

n = no, do not generate PATRAN files

prefix:

this will be the filename prefix that will be assigned to all PATRAN files.

☞ **Note:** This is only required if *patran* is yes

Example 1: (select PATRAN output, use file prefix "run1")

*PATRAN

y

run1

Example 2: (do not select PATRAN output)

* PATRAN

n

☞ **Note:** If this option is chosen, **MAC** generates the following PATRAN files:

- 1) ***prefix.patgeo***: contains "geometry" information of the RVE.
(this file is written in PATRAN 2.5 neutral file format in which the subcells are treated as "elements")
- 2) ***prefix.patstr***: contains stress quantities
(file is formatted as a PATRAN 2.5 element results file)
- 3) ***prefix.patepsin***: contains inelastic strain quantities
- 4) ***prefix.patepsto***: contains total strain quantities

For **Example 1**, the following files would be produced:

run1.patgeo
run1.patstr
run1.patepsin
run1.patepsto

4.3.11 Integrator Identification

Purpose: Select type of integration scheme

* *integrator comment*

ntf

* *initial time step comment*

istp

* *error tolerance comment*

errtol

ntf:

1 = Forward Euler method

2 = Predictor/Corrector method

istp:

= initial time step

errtol:

= error tolerance for predictor/corrector

☞ **Note:** *errtol* is only required when using predictor/corrector (*ntf* = 2)

Suggested errtol = 0.1

Example 1: (select predictor/corrector, with initial time step = 0.001 and error tolerance = 0.01)

*NTF

2

* ISTP

0.001

* ERRTOL

0.01

Example 2: (select forward euler, time step = 0.001)

* NTF

1

* ISTP

0.001

4.3.12 Constituent Material Model Identification:

Purpose: To select the model for the fiber and matrix constituents

* *material model comment*
ncmd

ncmd:

1 = Bodner-Partom Model

2 = Robinson Creep Model

3 = Robinson Non-normalized Viscoplastic Model

4 = Generalized Viscoplastic Potential Structure (GVIPS) Model

Example: (select Robinson Non-normalized Viscoplastic Model)

*NCMD

3

☛ **Note:** Currently all phases, e.g. both the fiber and matrix, constituents, must use the same material model.

☛ **Note:** See Section 3.3 for a mathematical description of each material model.

4.3.13 Number of different Materials:

Purpose: Define the total number of different materials

☛ **Note:** see below for the proper material constants required.

* number of materials comment

nmat

* material #1 comment

mdata

* database option comment

idb

:

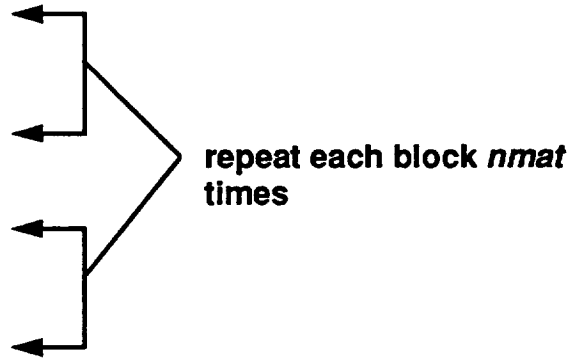
:

* material #*nmat* comment

mdata

* database option comment

idb



nmat - number of materials

mdata - material identification letter selected from material database below

MAC Isothermal Materials Database

Model (4.3.13)	Material	Units	<i>mdata</i>
Bodner-Partom <i>ncmd</i> = 1	Boron	MPa, sec	A
	Aluminum	" "	B
	SCS-6	" "	C
	Ti-15-3	" "	D
	Ti-6-4	" "	E
Robinson Creep <i>ncmd</i> = 2	Tungsten	ksi, hr	A
	Kanthal	" "	B
Robinson Viscoplastic <i>ncmd</i> = 3	Tungsten	ksi, hr	A
	Kanthal	" "	B
	FeCrAlY	" "	C
	Weak interface	" "	D
GVIPS <i>ncmd</i> = 4	TIMETAL21S	ksi, sec	A
	SCS-6	" "	B
	Weak interface	" "	C

idb - read material constants from the database (y) or read from mac.key file (n)

Note: if *idb* is n (no) then the following four lines **must** also appear:

* *dummy keyword*
elastic constants
 * *dummy keyword*
viscoplastic constants

Example: (select 2 materials, material 1: Boron, read from database , material 2: Aluminum, enter properites)

```
*NMAT
2
*MAT1
A
*IDB
y
*MAT2
B
*IDB
n
*ELASTIC
E, v, G,  $\alpha$  (see below for actual constants required)
*INELASTIC
a, b ,c ,d, ... (see below for actual parameters required)
```

Required Format for Isothermal Material Constants:

Bodner-Partom: *ncmd* = 1

<u>Elastic:</u>	<u>Inelastic:</u>
E, v	D_0, Z_0, Z_1, m, n, q

Robinson Creep: *ncmd* = 2

<u>Elastic:</u>	<u>Inelastic:</u>
$E_1, E_2, v_1, v_2, G_{12}, \alpha_1, \alpha_2$	$\sigma_0, \dot{\epsilon}_0, n, \beta, m, R, H$

Robinson Viscoplastic: *ncmd* = 3

<u>Elastic:</u>	<u>Inelastic:</u>
$E_1, E_2, v_1, v_2, G_{12}, \alpha_1, \alpha_2$	$n, m, \mu, \kappa_T, \beta, R, H, \hat{G}_0, \eta, \omega$

GVIPS: *ncmd* = 4

<u>Elastic:</u>	<u>Inelastic:</u>
E, v	$\mu, \kappa, R_\alpha, R_\kappa, B_0, B_1, L_0, L_1, m, n, p, q, w, z_0$

Non-isothermal Material Constants

The Following materials are available for a non-isothermal analysis:

MAC Nonisothermal Materials Database

Model (4.3.13)	Material	Units	<i>mdata</i>
Bodner-Partom <i>ncmd</i> = 1	Graphite	MPa, sec, ° C	A
	Aluminum	" "	B
	User Defined	" "	C

Required Format for Non-Isothermal Material Constants:

n_{tpts}

$T_1, T_2, \dots, T_{n_{tpts}}$

$E_{T_1}, E_{T_2}, \dots, E_{T_{n_{tpts}}}$

$v_{T_1}, v_{T_2}, \dots, v_{T_{n_{tpts}}}$

$G_{T_1}, G_{T_2}, \dots, G_{T_{n_{tpts}}}$

$\alpha_{T_1}, \alpha_{T_2}, \dots, \alpha_{T_{n_{tpts}}}$

$D_{0_{T_1}}, D_{0_{T_2}}, \dots, D_{0_{T_{n_{tpts}}}}$

$Z_{0_{T_1}}, Z_{0_{T_2}}, \dots, Z_{0_{T_{n_{tpts}}}}$

$Z_{1_{T_1}}, Z_{1_{T_2}}, \dots, Z_{1_{T_{n_{tpts}}}}$

$m_{T_1}, m_{T_2}, \dots, m_{T_{n_{tpts}}}$

$n_{T_1}, n_{T_2}, \dots, n_{T_{n_{tpts}}}$

$q_{T_1}, q_{T_2}, \dots, q_{T_{n_{tpts}}}$

Note: Currently, only the Bodner-Partom Model has nonisothermal constants.

4.3.14 RVE Identification:

Purpose: Select RVE representing desired fiber packing arrangement/architecture

* RVE comment

idp

idp:

- 1 = Square Fiber, Square Pack (original 4-cell model)

$$V_f \leq 1 / (1 + \Delta)^2$$

RVE shown in Fig. 5

- 2 = Square Fiber, Triangular (hexagonal) Pack

$$V_f \leq 0.86602 / (1 + \Delta)^2$$

RVE shown in Fig. 5

- 3 = Square Fiber, Square Diagonal Pack

$$V_f \leq 0.5 / (1 + \Delta)^2$$

RVE shown in Fig. 5

- 4 = Cross Shaped Fiber, Square Pack

$$V_f \leq 1 - 4 (xa)^2$$

RVE shown in Fig. 5

- 6 = Circular Fiber Approximation Rectangular or Square Pack

$$V_f \leq \frac{0.8125}{R (1 + \Delta)^2} \quad \text{if} \quad R > 1.0$$

$$V_f \leq \frac{R (0.8125)}{(1 + \Delta)^2} \quad \text{if} \quad R < 1.0$$

RVE shown in Fig. 5

- 9 = Two Different Size Square Fibers, Rectangular or Square Pack

$$V_{f_2} \leq \frac{1}{R \left[(1 + \Delta_2) + (1 + \Delta_1) \frac{R_{f_1}}{R_{f_2}} \right]^2}$$

$$V_{f_1} \leq \frac{2\sqrt{RV_{f_2}}}{\left[\left(\frac{R_{f_2}}{R_{f_1}} \right)^2 (1 + \Delta_2) + \left(\frac{R_{f_2}}{R_{f_1}} \right) (1 + \Delta_1) \right]}$$

RVE shown in Fig. 5

- 11 = Square Fiber, Rectangular Pack

$$V_f \leq \frac{1}{R(1 + \Delta)^2} \quad \text{if} \quad R > 1.0$$

$$V_f \leq \frac{R}{(1 + \Delta)^2} \quad \text{if} \quad R < 1.0$$

RVE shown in Fig. 5

- 99 = User Defined RVE
Example of RVE representing random packing shown in Fig. 6
Required input shown in Appendix D.

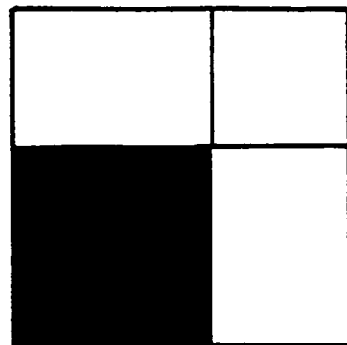
Example: (select RVE idp=1)

*RVE

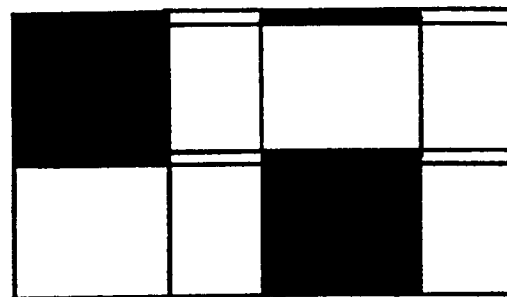
1

☞ **Note:** R , R_{f_1} , R_{f_2} , V_f , $\Delta = cper$, $\Delta_1 = cper1$ and $\Delta_2 = cper2$ are defined in sec. 4.3.16

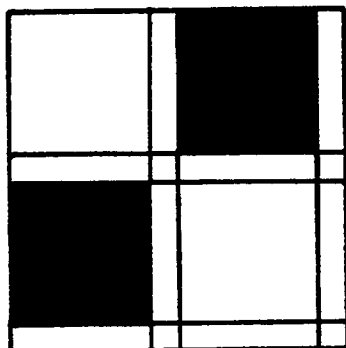
☞ **Note:** The images of the RVE's shown in Figs.5 and 6 were generated using the PAT-RAN option (section 4.3.11) available in **MAC**.



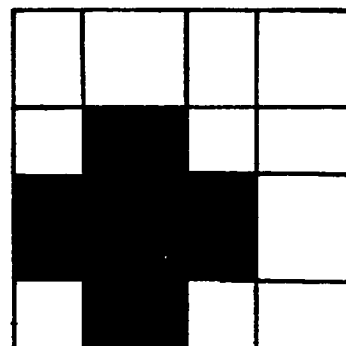
IDP = 1



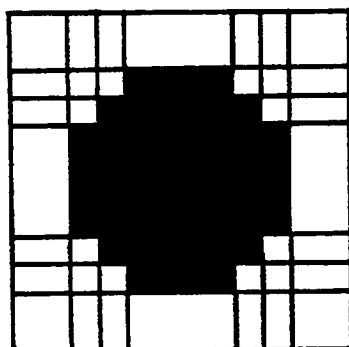
IDP = 2



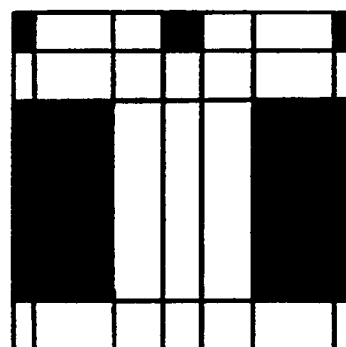
IDP = 3



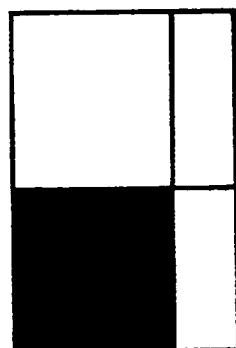
IDP = 4



IDP = 6



IDP = 9



IDP = 11

Matrix



Fiber



Figure 5: RVE's Available in *MAC*

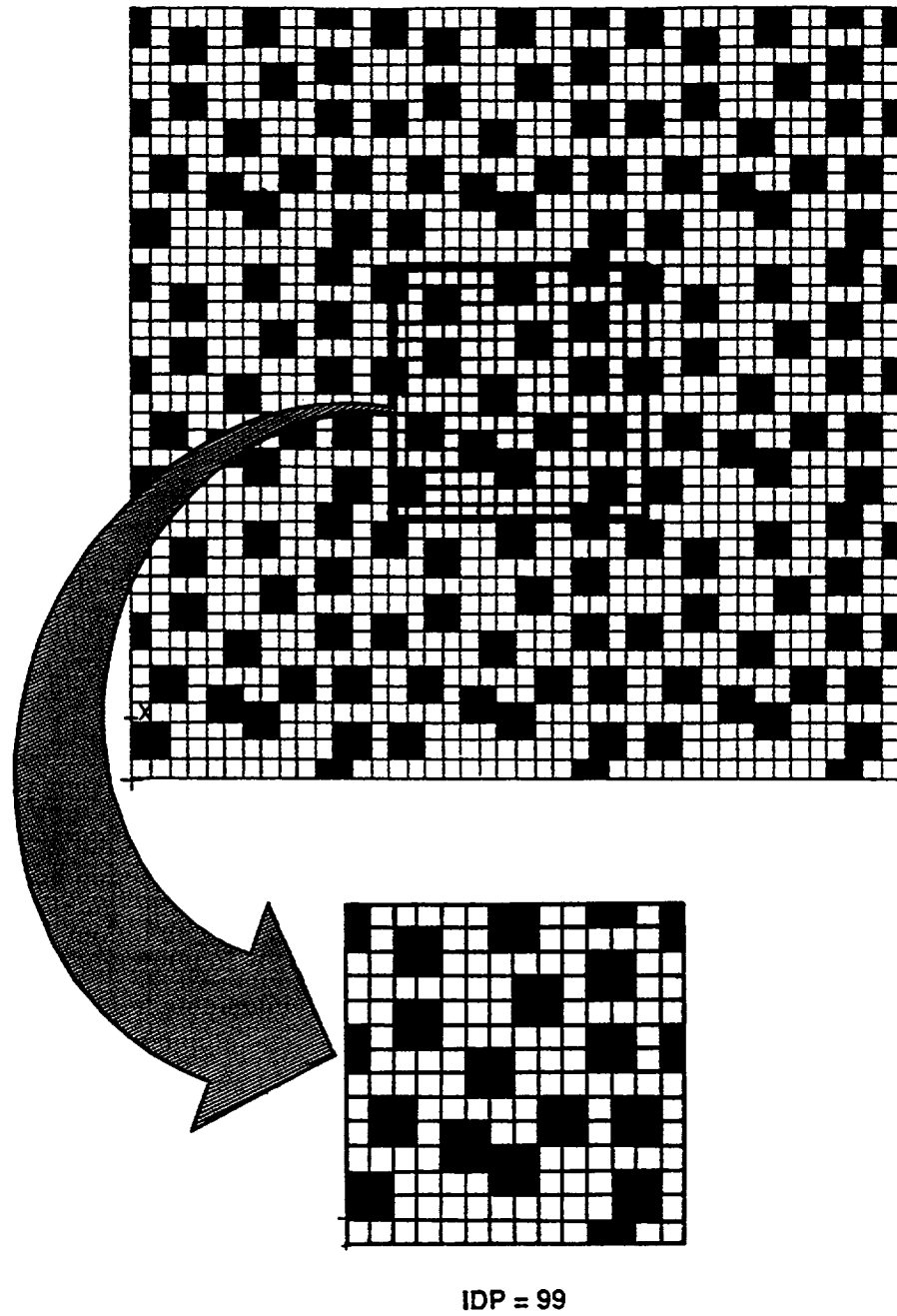


Figure 6: User defined RVE

4.3.15 Fiber/Matrix Interface Option:

** fiber/matrix interface comment*
inter

inter :
1 - with interface
2 - no interface

Example: (select interface option)
 *INTERFACE
 2

4.3.16 RVE Data:

Purpose: Enter required RVE data.

Without Interface: (inter=2)

- For IDP = 1, 2, 3
 - * *RVE comment*
 - vf*
- For IDP = 4
 - * *volume fraction comment*
 - vf*
 - * *xa distance comment*
 - xa*
- For IDP = 6
 - * *volume fraction comment*
 - vf*
 - * *side ratio comment*
 - R*
- For IDP = 9
 - * *volume fraction 1 comment*
 - vf1*
 - * *fiber radius 1 comment*
 - rad1*
 - * *volume fraction 2 comment*
 - vf2*
 - * *fiber radius 2 comment*
 - rad2*
 - * *side ratio comment*
 - R*
- For IDP = 11
 - * *volume fraction 1 comment*
 - vf1*
 - * *fiber radius 1 comment*
 - rad1*
 - * *side ratio comment*
 - R*
- For IDP = 99
 - * *RVE dimensions comment*
 - nb,ng*
 - * *h dimensions comment*
 - h₁, h₂, h_{ng}*
 - * *l dimensions comment*
 - l₁, l₂, l_{nb}*

With Interface: (inter=1)

- For IDP = 1, 2, 3
 - * fiber volume ratio comment
vf
 - * fiber radius 1 comment
rad1
 - * interface thickness comment
cper
- For IDP = 4
 - ☞ **Currently NOT Available**
- For IDP = 6
 - ☞ **Currently NOT Available**
- For IDP = 9
 - * fiber 1 volume ratio comment
vf1
 - * fiber radius 1 comment
rad1
 - * interface 1 thickness comment
cper1
 - * fiber 2 volume ratio comment
vf2
 - * fiber radius 2 comment
rad2
 - * interface 2 thickness comment
cper2
 - * side ratio comment
R
- IDP = 11
 - * fiber 1 volume ratio comment
vf1
 - * fiber radius 1 comment
rad1
 - * side ratio comment
R
 - * interface thickness comment
cper
- For IDP = 99
 - * RVE dimensions comment
nb,ng
 - * h dimensions comment
h₁, h₂, h_{ng}
 - * l dimensions comment
l₁, l₂, l_{nb}

where:

v_f, v_{f1}, v_{f2} = the fiber volume ratios

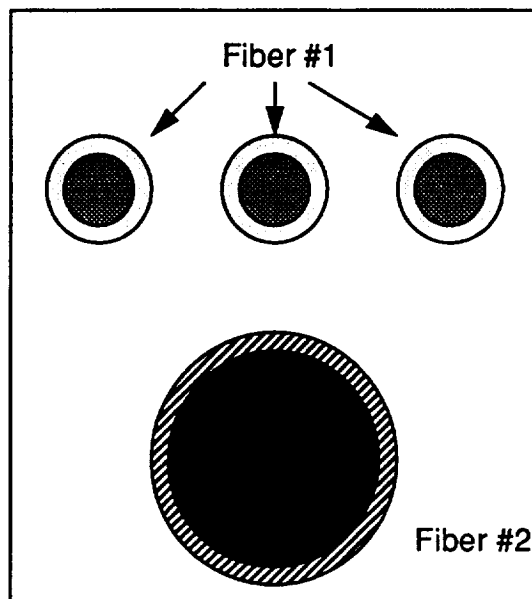
$rad, rad1, rad2$ = fiber radii

$c_{per}, c_{per1}, c_{per2}$ = ratios of interface thickness to fiber radius

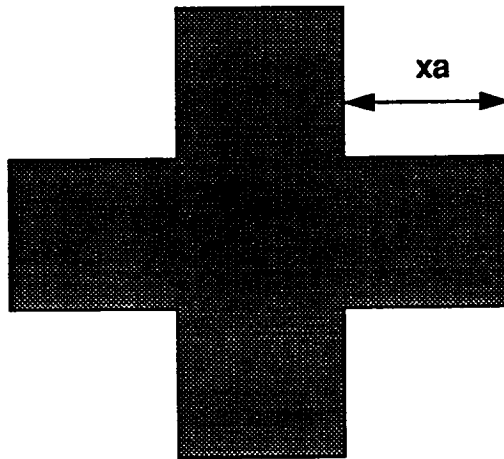
x_a = length of the cross

$R = X/Y$ which defines the ratio of distances between fiber within a "ply" and those between a "ply" (see figure on following page)

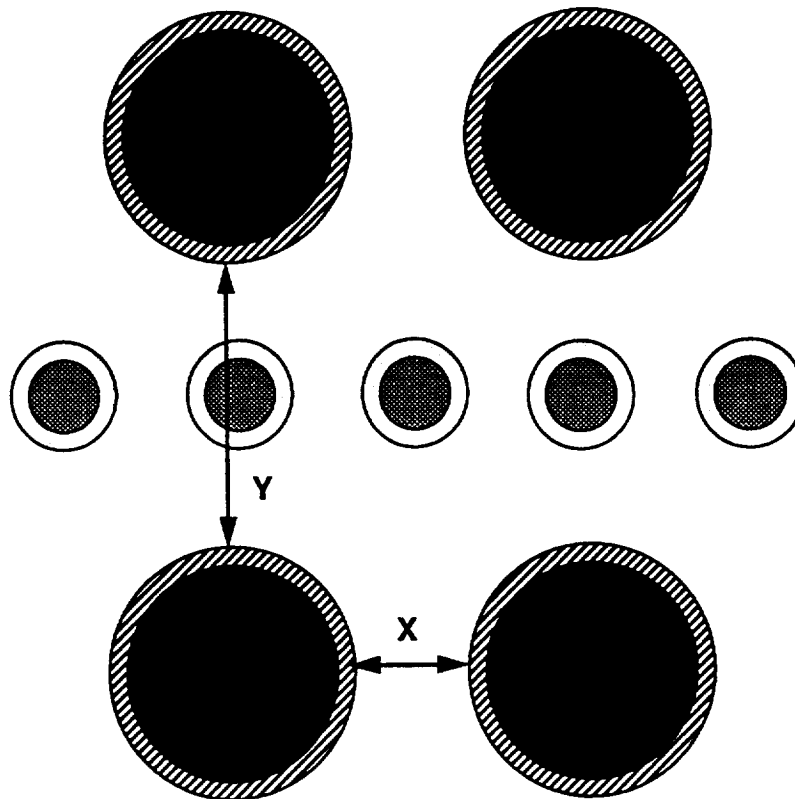
Hybrid Composite RVE



Cross Shaped Fiber Distance x_a



Fiber Spacing Ratio, $R=X/Y$



4.3.17 Plot Point Information:

Purpose: Specify the frequency at which data will be written to output files for both X-Y data and PATRAN if applicable. This provides the user with the ability to control the size of the output files since PATRAN files can become large, depending on the problem.

** plot point frequency comment
npmax*

Example: (print out every fifth data point)

```
*NPMAX  
5
```


4.3.18 Curve Data:

Purpose: Select plot variables for x and y axes and plot data filename

Specifying Curve Data For Macro (composite) Quantities:

* *curve 1 comment - (curve 1)*
 * *x variable comment - (x variable)*
maidx
 * *y variable comment - (y variable)*
maidy
 * *filename comment n- (filename)*
tname
 * *continuation comment - (more)*
more?

maidx and maidy variable options:

1 - e_{11}	7 - σ_{11}	13 - ϵ_{11}^i	19 - ϵ_{11}^{th}	22 - Total Time
2 - e_{22}	8 - σ_{22}	14 - ϵ_{22}^i	20 - ϵ_{22}^{th}	23 - Creep Time
3 - e_{33}	9 - σ_{33}	15 - ϵ_{33}^i	21 - ϵ_{33}^{th}	24 - Temperature
4 - γ_{12}	10 - τ_{12}	16 - γ_{12}^i		
5 - γ_{23}	11 - τ_{23}	17 - γ_{23}^i		
6 - γ_{13}	12 - τ_{13}	18 - γ_{13}^i		

tname:

--- = name of plot file

☛ **Note:** The file(s) generated will be of the form *tname_mac.data*. If the user desires to use the same *tname* for files 2-5, a double quote, "", is entered for *tname*. Those files then will have the form:

tname2_mac.data
tname3_mac.data
 etc.

(see the example for more details)

more?:

y = generate another data file
 n = finished selecting data files

☛ **Note:** Currently a maximum of 5 curves maybe specified per problem

EXAMPLE:

* CURVE 1

* X

1

* Y

7

* FILENAME

stress

file created: **stress_mac.data**

* MORE?

y

* CURVE 2

* X

22

* Y

13

* FILENAME

"

file created: **stress2_mac.data**

* MORE?

y

* CURVE 3

* X

23

* Y

13

* FILENAME

plot

file created: **plot_mac.data**

* MORE?

n

Specifying Curve Data for Micro (subcell) Quantities:

* *micro option comment*

micro

micro:

y = generate subcell data files

n = no subcell data requested

if micro is y (yes), then enter the following data lines:

* *number of subcells comment*

nucell

* *curve 1 comment - (curve 1)*

* *x variable comment - (x variable)*

miidx

* *y variable comment - (y variable)*

miidy

* *filename comment - (filename)*

tname2

* *dummy keyword*

more?

miidx and miidy:

1 - e_{11}	7 - σ_{11}	13 - ϵ_{11}^i	19 - Φ_{11}	25 - Ψ_{11}	31 - Total Time
2 - e_{22}	8 - σ_{22}	14 - ϵ_{22}^i	20 - Φ_{22}	26 - Ψ_{22}	32 - Creep Time
3 - e_{33}	9 - σ_{33}	15 - ϵ_{33}^i	21 - Φ_{33}	27 - Ψ_{33}	33 - Temperature
4 - γ_{12}	10 - τ_{12}	16 - γ_{12}^i	22 - Φ_{12}	28 - Ψ_{12}	
5 - γ_{23}	11 - τ_{23}	17 - γ_{23}^i	23 - Φ_{23}	29 - Ψ_{23}	
6 - γ_{13}	12 - τ_{13}	18 - γ_{13}^i	24 - Φ_{13}	30 - Ψ_{13}	

The quantities Φ and Ψ are the possible internal state variables (constitutive model dependent).

tname2:

--- = name of plot file

☞ **Note:** The file(s) generated will be of the form *tname2_mic.data*. If the user desires to use the same *tname2* for files 2-5, a double quote, " , is entered for *tname2*. Those files then will have the form:

tname22_mic.data
tname23_mic.data
etc.

(see the example for more details)

nucell:

--- = subcell number

more?:

y = to enter another subcell number

n = finished selecting subcells

EXAMPLE:

```
* MICRO?
y
* NUCELL
1
* CURVE 1
* X
1
* Y
7
* FILENAME
cell
* MORE?
n
```

file created: **cell_mic.data**

4.3.19 Multiple Run Option:

Purpose: Specify if a new “case” or “problem” is to be run

* case comment

ncase

* problem comment

nprob

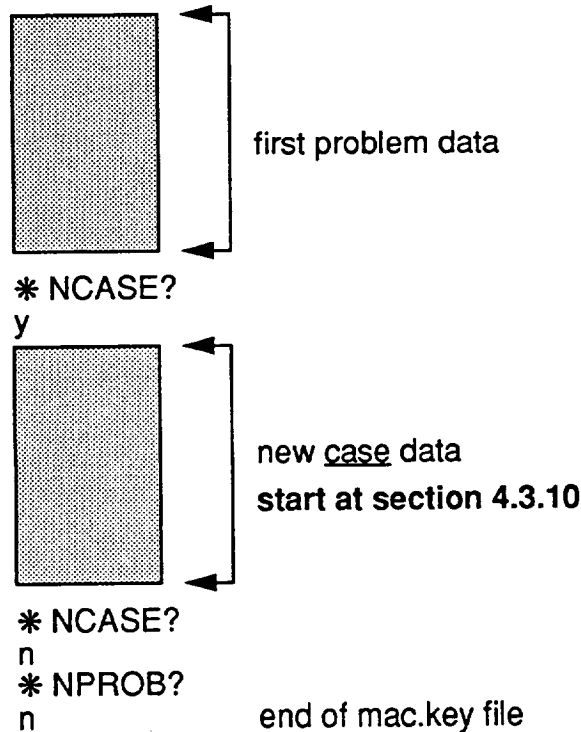
Example: *NCASE
 n
 *NPROB
 n

Note: Here, a new “case” means to run the problem with the same load type and history but with a new material model, new material constants, and/or RVE.

A new “problem” is similar to the above except that a new load type and history may also be specified.

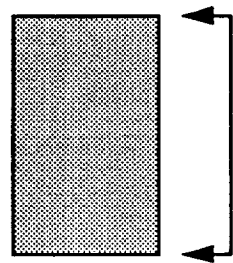
This option allows a sequence of runs to be made with different load types, load histories, material models, material constants, and packing arrangements all contained within a single MAC.key file

Note: if *ncase* is y then the data for the next case must follow, for example,



example of an additional case desired

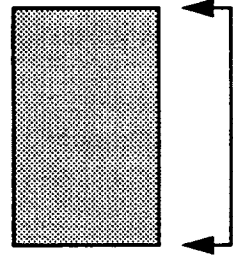
Note: if *ncase* is n but *nprob* is y then the following format is used,



first problem data

* NCASE?
n
* NPROB?
y

example of an
additional problem
desired



new problem data
start at section 4.3.4

* NCASE?
n
* NPROB?
n

end of mac.key file

Refer to Appendix B for a detailed mac.key file example.

5.0 Conclusion/Future Modifications

A computationally efficient, user-friendly, comprehensive, micromechanics analysis tool, **MAC**, has been presented that admits physically based viscoplastic deformation and life models, can analyze multiphased materials of interest in advanced propulsion systems, and can assist both the material scientist and structural analyst in developing, designing and analyzing strategic materials. However, the development of this tool is far from complete. A number of future enhancements that are planned and currently underway include:

- 1) Provide a convenient link for user definable constitutive material models.
- 2) Provide an implicit integration algorithm to improve computational efficiency.
- 3) The ability for each subcell to utilize a different material model.
- 4) The incorporation of damage evolution laws and failure criteria so as to provide life estimates.
- 5) The incorporation of lamination theory to allow analysis of laminates.

6.0 Appendix A

Sample mac.key File For A Mechanical Load Problem

The following example is used to explain the control blocks in more detail.

Problem Summary:

Load Type:	Mechanical
Load Component:	22-direction (transverse to fiber)
Load History:	Cyclic
Load Control:	Strain
Load History Data:	$\dot{\epsilon} = 8.333 \times 10^{-4}$, $\epsilon_{max} = 0.015$, $\epsilon_{min} = 0$. $\Delta t_{initial} = 0.0000024$
Micromechanics model:	Double Periodicity
Fiber Packing Arrangement:	Hexagonal Pack at 35% fiber volume ratio
Integration Algorithm:	Predictor/Corrector
Constituent Material Model:	GVIPS
Constituents:	Fiber: SCS-6 Matrix: TIMETAL21S Interface: fictitious weak interface for TIMETAL21S

*FOR MECHANICAL LOAD RUN	Header Line
*JRUN INTERACTIVE=1 BATCH=2 2	Batch Control Mode
*NPLVL -1	Print Level
*NSEL 2	Load Type: Mechanical
*LOP 2	Load component in 22-direction
*IOPT5 1	Strain Control
*NPTW 2	2 Data points
*TIMES 0.,18.	Time Data
*LOAD 0.,0.015	Load Data
*TREF 650.	Reference Temperature
*MODID 1	Double Periodicity
*NTF 2	Predictor/Corrector
*ISTP 0.0000024	Initial Step = 0.0000024
*ERRTOL 0.1E-2	Error Tolerance
*PATRAN n	No PATRAN Output
*NCMD 4	GVIPS Model
*NMT 3	3 materials

*MAT1 B *IDB y
*MAT2 A *IDB y
*MAT3 C *IDB n *ELASTIC 11700.,11700.,0.365,0.365,4287.5,1.,1. *VISCOPLASTIC 0.8E-8,0.1,0.1E-5,0.,0.85E-3,0.05,1.,1.,1.,3.3,1.8,1.35,1.,0.01
*IDP 2
*INTERFACE 1
*VF 0.35 *RAD 0.07 *CPER 0.1
*FIBID 1 *INTID 3 *MATID 2
*NPMAX 5
*CURVE 1 *X 2 *Y 8

Material 1: SCS-6

read from database

Material 2: TIMETAL21S

read from database

Material 3: Weak Interface

Read constants from key file

Elastic constants

Viscoplastic constants

RVE: Hexagonal Pack

Include fiber/matrix
Interface

Volume Fraction

Fiber Radius

Interface
Thickness/Fiber Radius

Fiber Material Id. = 1

Interface Material id. = 3

Matrix Material Id. = 2

Print requested data every
5 increments

Curve 1 data:

ϵ_{22}

σ_{22}

*FILENAME
SEtranwhex35

Filename for Curve 1

*MORE?

No more macro quantities

n

*MICRO?

No micro quantities

n

*NCASE?

No new cases

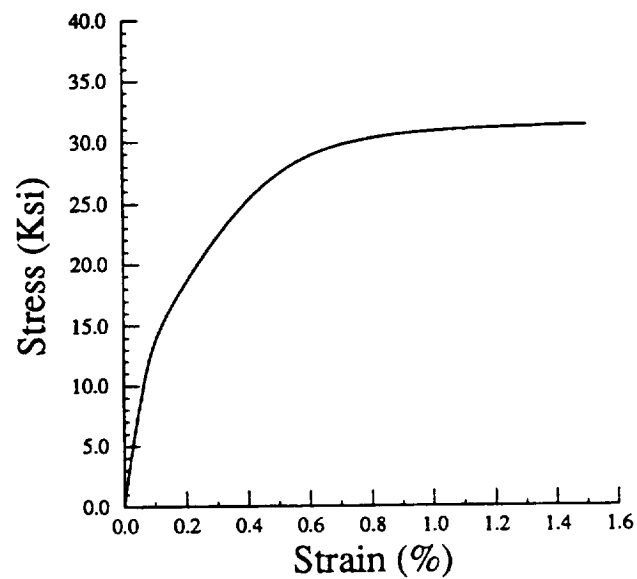
n

*NPROB?

No new problems

n

The following figure was obtained from the x-y plot data file produced by the present example.



Note: It is recommended that a new user construct a mac.key file using the data given in this appendix and then check to see if the same result plot is obtained.

7.0 Appendix B

Sample of A Series of Runs Contained Within One mac.key File

```
*FOR MECHANICAL LOAD RUN
*JRUN INTERACTIVE=1 BATCH=2
2
*NPLVL
-1
*NSEL
2
*LOP
2
*IOPT5
1
*NPTW
2
*TIMES
0.,12.0
*LOAD
0.,0.01
*TREF
873.
*MODID
1
*NTF
2
*ISTP
0.0048
*ERRTOL
0.1E-2
*PATRAN
n
*NCMD
4
*NMT
3
*MAT1
B
*IDB
y
*MAT2
A
*IDB
y
*MAT3
C
*IDB
n
*ELASTIC
1170.,1170.,0.365,0.365,4285.7,1.0,1.0
```

```

*VISCOPLASTIC
0.8D-7,0.1,0.1D-5,0.,0.85E-4,0.05,1.,1.,1.,3.3,1.8,1.35,1.,0.01
*IDP
1
*INTERFACE
1
*VF
0.35
*RAD1
0.07
*CPER
0.1
*FIBID
1
*INTID
3
*MATID
2
*NPMAX
1
*CURRE 1
*X
2
*Y
8
*FILENAME
test
*MORE?
n
*MICRO?
n
*NCASE?
y
*MODID ////////////////////////////////////////////////////
1
*NTF
2
*ISTP
0.0048
*ERRTOL
0.1E-2
*PATRAN
n
*NCMD
4
*NMT
3
*MAT1
B
*IDB
y
*MAT2
A

```

Select new case option

Beginning of new case data
Note that it begins at
section 4.3.10

```

*IDB
y
*MAT3
C
*IDB
n
*ELASTIC
11700.,11700.,0.365,0.365,4285.7,1.0,1.0
*VISCOPLASTIC
0.8D-7,1.,0.1D-5,0.,0.85E-4,0.05,1.,1.,1.,3.3,1.8,1.35,1.,0.01
*IDP
1
*INTERFACE
1
*VF
0.35
*RAD
0.07
*CPER
0.1
*FIBID
1
*INTID
3
*MATID
2
*NPMAX
1
*CURVE 1
*X
2
*Y
8
*FILENAME
test2
*MORE?
n
*MICRO?
n
*NCASE?
n
*NPROB?
y
*NSEL ///////////////////////////////////////////////////////////////////
2
*LOP
2
*IOPT5
1
*NPTW
2
*TIMES
0.,12.0

```

Skip new case option

Select new problem option

Beginning of new problem
data

Note that it begins at
section 4.3.4

```
*LOAD
0.,0.01
*TREF
873.
*MODID
1
*NTF
2
*ISTP
0.0024
*ERRTOL
0.10E-2
*PATRAN
n
*NCMD
4
*NMT
3
*MAT1
B
*IDB
y
*MAT2
A
*IDB
y
*MAT3
A
*IDB
n
*ELASTIC
1170.,1170.,0.365,0.365,4285.7,1.0,1.0
*VISCOPLASTIC
0.8D-7,0.1,0.1D-5,0.,0.85E-4,0.05,1.,1.,1.,3.3,1.8,1.35,1.,0.01
*IDP
1
*INTERFACE
1
*VF
0.35
*RAD
0.07
*CPER
0.1
*FIBID
1
*INTID
3
*MATID
2
*NPMAX
1
*CURRE 1
*X
```

MAC: Micromechanics Analysis Code

2
*Y
8
*FILENAME
test3
*MORE?
n
*MICRO?
n

*NCASE?
n
*NPROB?
n

End of mac.key file

8.0 Appendix C

Sample mac.key File For A Thermal Load Problem

The following example is used to explain the control blocks in more detail.

Problem Summary:

Load Type:	Thermal
Load History Data:	$\dot{T} = 0.01,$ $T_{max} = 371.1,$ $T_{min} = 21.1$ $\Delta t_{initial} = 17.505$
Micromechanics model:	Double Periodicity
Fiber Packing Arrangement:	Square Pack at 35% fiber volume ratio
Integration Algorithm:	Predictor/Corrector
Constituent Material Model:	Bodner-Partom
Constituents:	Fiber: Graphite Matrix: Aluminum

 **Note:** This problem is taken from reference 1., pg.238

*FOR MECHANICAL LOAD RUN

*JRUN INTERACTIVE=1 BATCH=2
2

*NPLVL
0

*NSEL
1

*NPTT
3
*TIMES
0.,35010.,70020.
*TEMPS
371.1,21.1,371.1

*TREF
371.1

*MODID
1

*NTF
2
*ISTPT
17.505
*ERRTOL
10.E-2

*PATRAN
n

*NCMD
1

*NMT
2

*MAT1
A
*IDB
y

*MAT2
B
*IDB
y

Number of Data Points

Time Data Points

Temperature Points

Predictor/Corrector

Initial step size

Error Tolerance

*IDP

1

*INTERFACE

2

*VF

0.3

*FIBID

1

*MATID

2

*NPMAX

5

*CURVE 1

*X

24

*Y

1

*FILENAME

thermal

*MORE?

n

*MICRO?

n

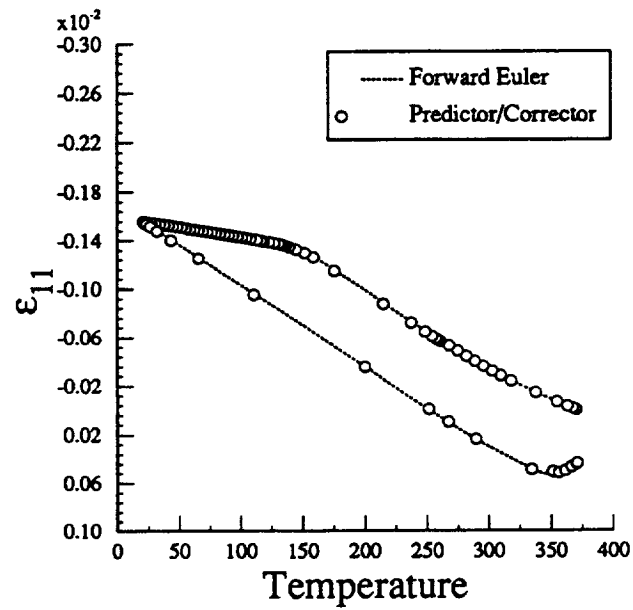
*NCASE?

n

*NPROB?

n

The following figure was obtained from the x-y plot data file produced by the present example.



Note: It is recommended that a new user construct a mac.key file using the data given in this appendix and then check to see if the same result plot is obtained.

9.0 Appendix D

Sample mac.key File For Random Composite

```

*FOR MECHANICAL LOAD RUN
*JRUN INTERACTIVE=1 BATCH=2
2
*NPLVL
-1
*NSEL
2
*LOP
1
*IOPT5
2
*NPTW
2
*TIMES
0.,0.04
*LOAD
0.,4.0
*TREF
873.
*MODID
1
*NTF
1
*ISTP
0.004
*PATRAN
n
*NCMD
3
*NMT
2
*MAT1
B
*IDB
y
*MAT2
D
*IDB
y
*IDP
99
*INTERFACE
2
*NB NG
14,14
*XH
1.,
1.,
1.,
1.,

```

```

1.,
1.,
1.,
1.,
1.,
1.,
1.,
1.,
1.,
1.,
1.,
*XL
1.,1.,1.,1.,1.,1.,1.,1.,1.,1.,1.,1.,1.
*MATNUM
1,2,2,2,2,2,1,1,2,2,1,1,2,1
1,2,1,1,2,2,1,1,2,2,2,2,1
2,2,1,1,2,2,2,2,2,1,1,2,2
2,2,2,2,2,2,1,1,2,1,1,2,2
2,2,1,1,2,2,2,1,1,2,2,2,2
1,2,1,1,2,2,2,2,2,1,1,2,1
1,2,2,2,2,1,1,2,2,2,1,1,2,1
2,2,2,2,2,1,1,2,2,2,2,2,2
2,1,1,2,2,2,2,1,1,2,1,1,2
2,1,1,2,1,1,2,2,1,1,2,1,1,2
2,2,2,2,1,1,1,1,2,2,2,2,2
1,1,2,2,2,2,1,1,2,2,2,1,1,2
1,1,2,2,2,2,2,2,2,2,2,1,1,2
2,2,2,2,2,2,2,2,2,2,1,1,2,2
*NPMAX
1
*CURVE 1
*X
1
*Y
7
*FILENAME
test
*MORE?
n
*MICRO?
n
*NCASE?
n
*NPROB?
n

```


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